3. CHEMICAL AND PHYSICAL INFORMATION

3.1 CHEMICAL IDENTITY

Barium is an alkaline earth metal of atomic number 56 in Group IIA of the periodic table of elements. It reacts with several other elements to form commercially-important salts. The chemical formula, structure, synonyms, and identification numbers for barium and its compounds are listed in Table 3-l.

3.2 PHYSICAL AND CHEMICAL PROPERTIES

Important physical and chemical properties of barium and its compounds are listed in Table 3-2.

TABLE 3-1. Chemical Identity of Barium and Compounds[a]

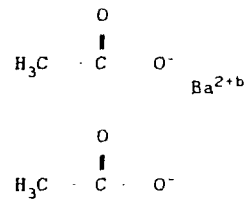
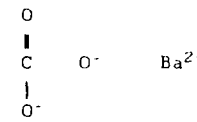
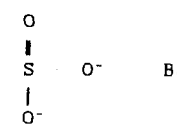
Characteristic	Barium	Barium acetate[b]	Barium carbonate
Synonyms	Elemental barium; barium ion; barium, alloys, non-pyrophoric; barium, alloys, pyrophoric; barium, metal, non-pyrophoric[c]	Acetic acid, barium salt; barium diacetate; barium acetate monohydrate[d,e]	Carbonic acid, barium salt; witherite[e,f]
Trade names	No data	No data	C.I. Pigment White 10; C.I. 77099[g]
Chemical formula	Ba; Ba^{2+}	$Ba(C_2H_3O_2)_2$; $Ba(CH_3CO_2)_2$; $Ba(CH_3CO_2)_2$[b,h,i]	$BaCO_3$
Chemical structure	Ba		
Identification numbers:			
CAS registry	7440-39-3	543-80-6[j]	513-77-9
NIOSH RTECS	CQ8370000	AF4550000[l]	CQ8600000[l]
EPA hazardous waste	D005[m]	No data	No data
OHM/TADS	7216597	No data	7216598
DOT/UN/NA/IMCO shipping	1339, 1400, 1854	No data	1564[c]
HSDB	4481	No data	950
NCI	No data	No data	No data

TABLE 3-1 (Continued)

Characteristic	Barium chloride	Barium cyanide	Barium hydroxide
Synonyms	Barium dichloride; barium chloride dihydrate[e,n]	Barium dicyanide	Barium dihydroxide; barium hydrate; barium hydroxide lime; barium hyroxide monohydrate; barium hydroxide octahydrate[b,n]
Trade names	SBA-0108E[l]	No data	Caustic baryta
Chemical formula	$BaCl_2$; $BaCl_2.2H_2O$[o]	BaC_2N_2; $Ba(CN)_2$[c]	$Ba(OH)_2$; $Ba(OH)_2.H_2O$; $Ba(OH)_2.8H_2O$[b,d]
Chemical structure	Ba^{2+} Cl^- Cl^-	Ba2+ C N[-b] C - N[-]	Ba^{2+} -OH[b] -OH
Identification numbers:			
CAS registry	10361-37-2	542-62-1	17194-00-2
NIOSH RTECS	CQ8750000	CQ8785000	No data
EPA hazardous waste	No data	P013	No data
OHM/TADS	7217223	7216599	7216600[p]
DOT/UN/NA/IMCO shipping	No data	1565	No data
HSDB	2633	403	1605
NCI	C61074[l]	No data	No data

TABLE 3-1 (Continued)

Characteristic	Barium oxide[b]	Barium sulfate	Barium sulfide[b]
Synonyms	Barium monoxide; barium protoxide[b,k]	Artificial heavy spar; artificial barite; barytes; blanc fixe; precipitated barium sulfate; sulfuric acid, barium salt[f,q]	No data
Trade names	No data	Baridol; CI 77120; CI Pigment White 21; Citobaryum; Enamel White; E-Z-Paque; Solbar; Steripaque	No data
Chemical formula	BaO[o]	$BaSO_4$	BaS[b]
Chemical structure	Ba ·· O[b]		Ba S[b]
Identification numbers:			
CAS registry	1304-28-5[j]	7727-43-7	21109-95-5[e]
NIOSH RTECS	CQ9800000[k]	CR0600000[l]	No data
EPA hazardous waste	No data	No data	No data
OHM/TADS	No data	No data	No data
DOT/UN/NA/IMCO shipping	No data	No data	No data
HSDB	No data	5041	No data
NCI	No data	No data	No data

[a]All information obtained from HSDB 1990 except where noted
[b]Windholz 1983
[c]DOT 1986
[d]Hawley 1981
[e]Sax and Lewis 1989
[f]EPA 1985c
[g]Hayes 1982
[h]Weast 1989
[i]Perry and Chilton 1973
[j]Sax and Lewis 1987
[k]Sax and Feiner 1984
[l]RTECS 1989
[m]EPA 1980a
[n]Kirkpatrick 1985
[o]Parmeggiani 1983
[p]OHM/TADS 1989
[q]Kunesh 1985

CAS = Chemical Abstracts Services; DOT/UN/NA/IMCO = Department of Transportation/United Nations/North America/International Maritime Dangerous Goods Code; EPA = Environmental Protection Agency; HSDB = Hazardous Substances Data Bank; NCI = National Cancer Institute; NIOSH = National Institute for Occupational Safety and Health; OHM/TADS = Oil and Hazardous Materials/ Technical Assistance Data System; RTECS = Registry of Toxic Effects of Chemical Substances

TABLE 3-2. Physical and Chemical Properties of Barium and Compounds[a]

Property	Barium	Barium acetate	Barium carbonate
Molecular weight	137.3	255.45	197.37
Color	Silver-white	White	White
Physical state	Malleable metal[e]	Crystals	Heavy powder or crystals[c]
Melting point	710°C[c]; 725°C	41°C (monohydrous)[b]	1740°C (α form, at 90 atm)
Boiling point	1600°C[c]; 1640°C	No data	Decomposes at 1300°C
Density	3.51 g/cm^3 (at 20°C)	2.468 g/cm^3 (anhydrous); 2.19 (monohydrous)[b]	4.25 g/cm^3[h]
Specific gravity	3.5 (at 20°C)[f]	2.02 (below 24.7°C)[h]	4.43
Odor	No data	No data	Odorless[i]
Odor threshold:	No data	No data	No data
Solubility:			
Water	Decomposes (temperature unspecified)[g]	588 g/L (at 0°C)[h]; 750 g/L (at 100°C, monohydrous)[b]	0.025 g/L (temperature unspecified)[c]; 0.022 g/L (at 18°C)[j]; 20 mg/L (at 20°C); 0.0065 pph and 60 mg/L (at 100°C)
Organic solvents			
Alcohol		1 g/700 mL[c]	Insoluble
Benzene	Soluble	No data	No data
Partition coefficients	Insoluble No data	No data	No data
Vapor pressure	10 mmHg (at 1049°C)[g]	No data	Essentially zero[k]
Henry's law constants	No data	No data	No data
Autoignition temperature	No data	No data	No data
Flashpoint	No data	No data	No data
Flammability limits	Explosion hazard if exposed to moist air[f]	No data	Nonflammable[i]
Conversion factors	No data	No data	No data
Explosive limits	No data	No data	No data

TABLE 3-2 (Continued)

Property	Barium chloride	Barium cyanide	Barium hydroxide
Molecular weight	208.27 (anhydrous); 244.31 (dihydrous)[b]	189.40	171.38[c]; 315.48 (octahydrous)[d]
Color	Colorless	White	White[c]
Physical state	Flat crystals[c]	Crystalline powder[c]	Powder[c]
Melting point	Transition at 925°C to cubic crystals (anhydrous)[l]; 960°C (anhydrous)[m]; 1130°C (dihydrous)[d]	No data	408°C (anhydrous)[e]; 78°C (octahydrous)[d]
Boiling point	1560°C (at 760 mmHg)	No data	780°C[d]; 550°C (octahydrous)[b]
Density	3.86 g/cm^3 (at 24°C)	No data	3.743 g/cm^3[c]
Specific gravity	3.1[h]	No data	2.18 (at 16°C)[f]; 4.495 (anhydrous)[b]
Odor	Odorless[k]	No data	No data
Odor threshold:	No data	No data	No data
Solubility:			
Water	375 g/L (at 26°C)[f]	800 g/L (at 14°C)	16.7 g/L (at 0°C)
Organic solvents			
Alcohol	Soluble in methanol	18 g/100 cm^3	Soluble
Partition coefficients	No data	No data	No data
Vapor pressure	Essentially zero[k]	No data	No data
Henry's law constants	No data	No data	No data
Autoignition temperature	No data	Nonflammable	No data
Flashpoint	No data	Nonflammable	No data
Flammability limits	No data	Nonflammable	No data
Conversion factors	No data	No data	No data
Explosive limits	No data	No data	Explosive > 216°C[n]

TABLE 3-2 (Continued)

Property	Barium oxide	Barium sulfate	Barium sulfide
Molecular weight	153.36	233.4	169.4
Color	White to yellowish-white[c]	White or yellowish	Grayish-white or pale yellow
Physical state	Powder or crystals	Crystals	Powder
Melting point	1920°C[c]; Decomposes at 400°C	1580°C (decomposes)[b]	1200°C; >2000°C
Boiling point	2000°C[k]	1149°C (monoclinical transitition point)[d]	Decomposes
Density	2.7 g/cm^3; 5/7 g/cm^3[c]	4.50 g/cm^3	4.25 g/cm^3
Specific gravity	5.72 (cubic)[h]	No data	No data
Odor	Odorless[k]	Odorless[c]	Sulfurous
Odor threshold	No data	No data	No data
Solubility:			
Water	1500 g/L (at 0°C)[b]; 908 g/L (at 80°C)[b]	0.00115 g/L (at 0°C)[m]; 0.00413 (at 100°C)	Decomposes (at 0°C)
Organic solvents			
Alcohol	Soluble[c]	Insoluble[d]	Insoluble
Partition coefficients	No data	No data	No data
Vapor pressure	Essentially zero[k]	No data	No data
Henry's law constants	No data	No data	No data
Autoignition temperature	No data	No data	No data
Flashpoint	No data	No data	No data
Flammability limits	Produces heat on contact with water or steam[k]	No data	Flammable by spontaneous chemical reactions[l]
Conversion factors	No data	No data	No data
Explosive limits	Contact with CO_2 or H_2S may cause explosion[l]	Heating with aluminum may cause violent explosions.	Air, moisture, or acid fumes may cause it to ignite[l]

[a]All references are to Weast 1989 unless otherwise specified.
[b]Perry and Chilton 1973
[c]Windholz 1983
[d]Parmeggiani 1983
[e]Hawley 1981
[f]Stokinger 1981
[g]EPA 1984
[h]Kirkpatrick 1985
[i]DOT 1986
[j]Meister 1989
[k]NIOSH/OSHA 1978
[l]Sax and Lewis 1989
[m]EPA 1987d
[n]HSDB 1989